REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)

2. REPORT DATE: Sept. 15, 1994

3. REPORT TYPE AND DATES COVERED: Final 15 Feb. 94 - 14 Feb. 95

4. TITLE AND SUBTITLE: Third International Workshop on Computational Electronics

5. FUNDING NUMBERS: 3145025---01

6. AUTHOR(S): Stephen M. Goodnick

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES):
Oregon State University
Department of Electrical & Computer Engineering
Corvallis, OR 97331-3211

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES):
Ms. June A. Hawley, Admins. Grants Officer
University of Washington
410 University District Building
Seattle, WA 98105-4631

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

The Third International Workshop on Computational Electronics (IWCE) was held at the Benson Hotel in downtown Portland, Oregon, on May 18, 19, and 20, 1994. The workshop was devoted to a broad range of topics in computational electronics related to the simulation of electronic transport in semiconductors and semiconductor devices, particularly those which use large computational resources. The workshop was supported by the National Science Foundation (NSF), the Office of Naval Research and the Army Research Office, as well as local support from the Oregon Joint Graduate Schools of Engineering and the Oregon Center for Advanced Technology Education. There were over 100 participants in the Portland workshop, of which more than one quarter represented research groups outside of the United States from Austria, Canada, France, Germany, Italy, Japan, Switzerland, and the United Kingdom. There were a total 81 papers presented at the workshop, 9 invited talks, 26 oral presentations and 46 poster presentations. The emphasis of the contributions reflected the interdisciplinary nature of computational electronics with researchers from the Chemistry, Computer Science, Mathematics, Engineering, and Physics communities participating in the workshop.

14. SUBJECT TERMS: Semiconductor transport, Computational electronics, device simulation,

15. NUMBER OF PAGES: 6

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
unclassified	unclassified	unclassified	none

NSN 7540-01-280-5500

Standard Form 298 (Rev 2-89)
Prescribed by ANSI Std. Z39-18
298-102

53-8

Third International Workshop on Computational Electronics

Stephen M. Goodnick
Department of Electrical and Computer Engineering
Oregon State University
Corvallis, OR 97331

The Third International Workshop on Computational Electronics (IWCE) was held at the Benson Hotel in downtown Portland, Oregon, on May 18, 19, and 20, 1994. The workshop was devoted to a broad range of topics in computational electronics related to the simulation of electronic transport in semiconductors and semiconductor devices, particularly those which use large computational resources. The workshop was supported by the National Science Foundation (NSF), the Office of Naval Research and the Army Research Office, as well as local support from the Oregon Joint Graduate Schools of Engineering and the Oregon Center for Advanced Technology Education. The present workshop has evolved from earlier workshops held at the Beckman Institute in Urbana-Champaign under the auspices of the NSF National Center for Computational Electronics (NCCE) located at the University of Illinois. Two earlier NCCE Computational Electronics workshops were held in 1990 and 1991, both at the Beckman Institute, and involved primarily members of the NCCE. In 1992 it was decided to expand the scope of the NCCE workshop to become an international forum for the discussion of current trends and future directions of computational electronics, and thus the First International Workshop on Computational Electronics was held on May 28-29, 1992, at the Beckman Institute. The following year, the 2nd IWCE was held at the University of Leeds in the United Kingdom on August 11-13, 1993.

There were over 100 participants in the Portland workshop, of which more than one quarter represented research groups outside of the United States from Austria, Canada, France, Germany, Italy, Japan, Switzerland, and the United Kingdom. The emphasis of the contributions reflected the interdisciplinary nature of computational electronics with researchers from the Chemistry, Computer Science, Mathematics, Engineering, and Physics communities participating in the workshop.

There were a total 81 papers presented at the workshop, 9 invited talks, 26 oral presentations and 46 poster presentations. The papers were organized into five sessions related to current topics in computational electronics:

1) Particle Simulation and other Boltzmann Equation Solution Methods

2) Hydrodynamic and other Expansion Methods for Device Modeling

3) Quantum Transport and Quantum Devices

4) High Performance Computing and Algorithms

5) Modeling of Optical Processes and Optoelectronic Devices

The conference began on Wednesday, May 18th with the session on particle simulation methods starting with an invited talk by Jack Higman from the Motorola Research and Development Laboratory in Austin, Texas. He reported on an ongoing study began several years ago through the NCCE to calibrate the results of Monte Carlo simulations from various groups around the world applied to the same problem, that of the distribution function in bulk Si at various electric field strengths. When preliminary results of this comparison were first reported by Massimo Fischetti from IBM Thomas Watson at the 1rst IWCE meeting in 1992, there was no apparent agreement between the results by various groups, particularly at the highest electric fields considered. This result was quite justly the source of a great deal of consternation among practitioners, particularly since Monte Carlo solutions are routinely used as the 'exact solution' to which approximate methods such as the hydrodynamic model are compared. A more thorough examination of the results of various groups reported by Jack Higman showed that the disagreement could to a large extent be traced to the underlying band structure model used by each group. Thus, groups that utilized basic effective mass models (nonparabolic bands) tended to converge to one set of results while groups that employed more sophisticated full band structure codes showed surprising convergence to a second set of results, even at the highest fields considered. The difference between effective mass models and full band structure models at high electric fields is not surprising given the increasingly poor representation of the actual band structure in the effective mass model as the electron energy increases. The results of this study reinforce the necessity of agreeing on a standard set of band structure parameters and electron-phonon coupling constants for researchers engaged in kinetic equation level modeling. A second invited talk in the same session by Kenji Taniguchi of Osaka University also addressed the issue of high field transport in Si using Monte Carlo simulation. The focus of this talk was the impact ionization process in Si which is a critical issue in submicron devices and device degradation due to hot electron effects. A full band structure simulation was reported which included a complete calculation of the impact ionization coefficient rather than relying on more approximate schemes such as the Keldysh approach, and excellent agreement reached with the impact ionization data in Si from the IBM group. Presentations by Neil Goldsman from Maryland and Alfred Kriman from SUNY, Buffalo also addressed the issue of impact ionization in device simulation. The latter group focussed on techniques to enhance rare statistical events during Monte Carlo simulation as did a presentation by Amanda Duncon from the Beckman Institute in the context of modeling submicron MOSFETs. Peter Rambo and William Lawson from Lawrence Livermore Laboratories reported on specific aspects of the Monte Carlo algorithm, the former re-examining the time step requirement in device simulation in comparison to the inverse plasma frequency, while William Lawson introduced a self-scattering technique in full band Monte Carlo for selecting final states efficiently. Other papers in this session dealt primarily with solutions to the Boltzmann transport equation (BTE) by alternate means than Monte Carlo methods. These included further results of device simulation using Cellular Automata techniques by Achim Rein from the Walter Schottky Institute in Munich, and the use of the scattering matrix method presented Carl Huster of Purdue University. A somewhat similar approach to the scattering matrix approach called the 'scattered packet method' was introduced by Luca Varani representing the Montpellier group, while Christoph Jungeman of the University of Aachen presented a correlation function analysis of the BTE based on a spherical harmonics expansion method. Noise and small signal analysis of the BTE via Monte Carlo and perturbation techniques was reported by the Montpellier group in collaboration with the University of Modena, Italy. A new algorithm for solving the time dependent BTE for electrons with that for nonequilibrium phonons was also presented by Peter Kocevar from the University of Graz in collaboration with the Montpellier and Modena groups. Process modeling by Monte Carlo methods was also reported by QuinSheng Zhang of Oregon State.

The second session of the workshop was devoted primarily to the hydrodynamic (HD) model obtained from moment expansion of the BTE. By including higher moments than the standard drift-diffusion model, generally in the form of an energy balance equation, non-local and nonstationary effects are built into the phenomenological device equations which require much less computation time than Monte Carlo solution of the BTE. As device dimensions continue to decrease, this model has demonstrated increased accuracy compared to the drift-diffusion model, which explains its current popularity in the device community. A general expansion formalism for the BTE was reported by Christian Ringhofer from Arizona State University which contains the HD model as the leading terms, and provides a mathematical basis for evaluating the validity of the HD approach for various applications. Wolfgang Fichtner of the Swiss Federal Institute of Technology was the invited speaker for this session, and his presentation related to the extensive work being carried out at Zurich on three dimensional modeling of semiconductor devices and processing for Technology Computer Aided Design (TCAD). One emphasis of the talk was the choice of appropriate computer architecture for large scale 3D HD device modeling. Detailed comparison of the performance of 3D algorithms on various parallel processing environments was reported on platforms ranging from distributed workstation clusters to distributed memory MIMD multiprocessor computers. A key issue observed by them was the communication latency of different architectures, which in some cases was so severe that the performance of certain parallel supercomputers was not noticeably improved compared to distributed computing on networked workstations (which cost substantially less). 3D HD modeling of submicron MOSFETs was also reported by Neil Goldsman from the University of Maryland using an iterative scheme to reduce the memory requirements and thus allow 3D modeling in a workstation environment. Jing-Rong Zhou of Arizona State University also presented a 3D device HD model of ultrasmall GaAs devices including quantum corrections based on the so called quantum hydrodynamic model which was introduced at the previous Leed's meeting. A new innovation was the inclusion of the potential of individual randomly distributed ionized donors in the simulation. Their results for short gate width and gate length devices showed 20 to 30% variations in the saturated current of devices with nominally identical dopings, but different random impurity configurations. A number of presentations dealt with the issue of modeling of heterojunction devices such as HFETs and HBTs. Implementation of a duel energy transport model into the latest release of PISCES-2ET was reported by the Zhiping Yu of Stanford University. 2D modeling of HFETs was reported by the University of Leeds group and by Scientific Research Associates, the latter also including quantum corrections. Presentations by Emad Fatemi from Lausanne and Rahim Khoie of the University of Nevada addressed specifically the simulation of transport over heterojunction barriers, and their inclusion in the HD equations. Simple analytic models for tunneling through heterojunction barriers in HBTs was considered by the group from the University of British Columbia. An investigation of the effects of heavy doping was reported by the University of Leeds. Further improvements in HD modeling of Si devices were also reported at the workshop. A hierarchial simulator for Si MOSFET simulation was presented by Srinivas Jallepalli from the University of Texas, Austin containing several levels of simulation ranging from drift-diffusion through HD and Monte Carlo simulation. Ting-Wei Tang of the University of Massachusetts presented an improved HD model for Si and SOI MOSFETs, as well as one for BJT modeling including viscous effects. The modeling group at Silvaco reported on a Si BJT model which included lattice heating effects in addition to the energy balance model which showed improved breakdown simulation in these devices. n^+-n-n^+ diode simulation was reported by groups at Wayne State University and the Stevens Institute of Technology. Finally, in connection with TCAD, the Stanford group presented a device parameter extractor for fitting equivalent circuit models from simulated device data.

An active area of current research is the study of ultra-small electronic devices where quantum phenomena are important. The quantum mechanical wave nature of the electrons gives rise to new physical effects, and much work is aimed at exploiting these phenomena for novel device applications. The modeling of quantum devices is a challenging task, both in formulating the problem and in solving the equations. Papers in this session addressed both aspects. In the phase coherent regime, electron dynamics is governed by the Schrodinger equation which is a wave equation for the electronic wave function. Craig Lent from the University of Notre Dame addressed in an invited presentation modeling issues for the case of coherent quantum transport. A specific device design of a quantum waveguide coupler was discussed by Massimo Macucci and coworkers at the Beckman Institute of the University of Illinois. The Notre Dame group presented an eigenvalue method to locate resonance peaks for electronic transmission in such quantum waveguide systems, as well as features of magnetotransport which are related to the Quantum Hall Effect. The electron mobility in these quasi-one-dimensional quantum wires is expected to be higher than in bulk due to the reduced dimensionality. However, electronic scattering events due to imperfections have a deleterious effect. The role of impurities and structural imperfections was addressed by David Ting from the California Institute of Technology, and by a collaborative effort between Oxford University and Oregon State University. Several papers concentrated on the electron-phonon interaction in quantum wires, such as contributions by researchers at Osaka University, Wayne State University, and the University of California at Berkeley. The self-consistent solution of the Poisson and Schrodinger equations was the topic of several presentations, such as the improved algorithm by S. Subramaniam of Oregon State University. Resonant tunneling structures are the basis of the fastest electronic devices, and their intrinsic high-frequency characteristics was the subject of a paper by the group at the University of Texas at Dallas. Several contributions addressed the problem of quantum transport beyond the Schrodinger equation picture. The loss of phase coherence due to the Coulomb interaction was discussed by Walter Potz of the University of Illinois at Chicago. In an invited presentation, Supriyo Datta of Purdue University summarized the work of his group on quantum device simulation including interaction, which is based on a non-equilibrium Green function approach. This was also the topic of presentation by Roger Lake of Texas Instruments, and by Felix Buot of the Naval Research Laboratory. Researchers of the University of Texas at Austin used a Wigner-Poisson model to study AlAs/GaAs resonant-tunneling diodes.

An issue of great importance in the computational electronics community are efficient numerical algorithms for high speed performance, particularly those which utlilize high performance computing such as vector or parallel environments. The Thursday afternoon session was devoted to this topic beginning with an invited talk by William Coughran of AT&T Bell Laboratories who reported on distributed computing algorithms for the drift-diffusion model using workstation clusters connected together through high speed data networks. A second invited talk in the same session was given by L. Ridgeway Scott of the University of Houston who discussed parallel iterative algorithms for solving elliptic partial differential equations such as one encounters in the standard drift-diffusion model. He reported on efficient algorithms with excellent parallel to sequential speedup for 3D simulation of semiconductor devices on both shared memory and distributed memory machines. Two other papers addressed parallel implementation of GaAs MESFET simulations, both from the group at the University of Leeds. Several other papers in this session addressed advanced algorithms related to solving the HD equations. Anand Pardhanani of the University of Austin reported on adaptive grid and multigrid techniques while Mario Ancona reported a new flux-corrected transport algorithm in semiconductor device simulation used previously for fluid dynamics simulation. Chi-Wang Shu from Brown University reported the conditions for the validity of using shock capturing algorithms in solving the HD model.

The final session of the workshop was devoted to modeling and simulation of optical processes and optical devices. Optical processes typically refer to ultrafast photoexcitation in semiconductor structures in which a strong optical field induces electron-hole pairs on very short time scales. Fausto Rossi from the University of Marburg was the invited speaker on this topic. His talk dealt with a novel particle simulation method for solving the coupled electron-hole dynamics with the coherent polarization of the medium induced by the ultrafast source. Such effects are important on time scales of 10s of femtoseconds which are now being probed by ultrafast lasers. In a related topic, Novat Nintunze of Washington State University reported on the effects of including dynamic screening into Monte Carlo simulations of photoexcited carriers in GaAs. Steven Durbin from Purdue University presented modeling of the emission spectrum from time resolved photoluminescence as well. Optical devices include semiconductor lasers, photodetectors, and display devices. Simulation of optical devices is an emerging subfield in the computational electronics community and one that is expected to grow substantially in the future. Jeff Scott of the University of Santa Barbara gave an overview presentation of the design and modeling of vertical-cavity surface-emitting lasers. This invited talk outlined problems which must be addressed in simulating such complicated structures which include size quantization of the electronic states, 3D effects, and solution of the electromagnetic problem of the fields in the cavity just to mention a few. There were a number of other papers which addressed the problem of simulation of semiconductor lasers. Three separate presentations from the University of Illinois group dealt with specific aspects of the physics of laser simulation related to ongoing work on a 2D self-consistent laser simulator MINILASE. Muhammad Alam from Purdue University also reported on laser modeling based on the scattering matrix approach presented in the first session of the workshop. Yijun Cai from the Oregon Graduate Institute presented numerical modeling of carrier confinement in quantum well lasers as well. Two presentations, one by Shankar Pennathur from Oregon State University and John Fogarty from the Oregon Graduate Institute discussed Monte Carlo modeling of AC thin film electroluminescent devices used in flat panel displays in which hot electron impact excitation of phosphorescent impurities is the mechanism responsible for light emission. The Lawrence Livermore group reported simulations of filament formation and propagation in photoconducting switches well.

As a major theme for this years meeting was modeling of semiconductor devices below 0.1 microns. To emphasize this theme, a one hour panel discussion composed of international experts in advanced device modeling was held on Wednesday evening, May 18th. The purpose was to provide a meaningful discourse on the limits of conventional device simulation techniques as critical device dimensions approach 100 nm and below, and to help define a roadmap of device CAD into the next decade. The panel was organized by Steve Laux of IBM Thomas Watson who acted as moderator and included David Ferry, Wolfgang Fichtner, Karl Hess, Kent Smith from AT&T Laboratories, Murray Hill, and Kenji Taniguchi. Based on the assumption that conventional device technology (i.e. Si MOSFETs) will continue to scale well below 0.1 microns, the panel was asked to address the question of to what limit the semiclassical paradigm holds, when do quantum effects become important, what new device concepts will have to be addressed, and what is the role of device modeling. There seemed to be general agreement with the statement by Kenji Taniguchi that below 0.1 microns in the absence of quantum interference phenomena that direct solution of the BTE including full band effects will be necessary for critical regions of the device, but that such solutions may be coupled with the less numerically intensive hydrodynamic model in other regions. However, there was not a general consensus on

when the classical model fails. David Ferry argued that quantum interference effects may even be important in present deep submicron devices in effects such as impurity scattering. Further, below 0.1 micron in ultrasmall devices, one must account for the exact locations of donors and acceptors as demonstrated by calculations presented during the hydrodynamic session discussed earlier, and drift-diffusion calculations performed at IBM. Large fluctuations in the DC characteristics are possible with different spatial configurations of donors for example in MESFETs with the same nominal doping density. Wolfgang Fichtner pointed out that IC process modeling lags in maturity at least 5 years behind that of transport modeling which limits our knowledge of the exact device structure to actually model. This problem becomes increasingly important as device dimensions scale which makes the task of simulation of production devices difficult. This point raised an interesting audience discussion on the actual role of device simulation in IC CAD. Clearly the goal of providing simulation tools accurate to a few percent and able to predict with the same level of accuracy the performance each new generation of device technology has eluded researchers thus far. Rather, device simulation has played the role of solving problems in existing technology, or providing the context for understanding the physics of device behavior. However, device technology itself often outpaces the applicability of simulation tools and will probably continue to do so. It was generally agreed that the juggernaut of semiconductor device technology will continue into the sub 0.1 micron regime, and that problems such as those posed by David Ferry will probably be overcome as have been every previous problem which supposedly put lower limits on the dimensions of semiconductor devices. The future challenge of Computational Electronics is to play a more active role in solving such problems, which as evidenced by the panel discussion, will require a much more thorough integration of process as well as device transport modeling and simulation.
The proceedings of the 3rd IWCE were published in August, 1994 by Oregon State University. Copies are available upon request at a cost of $35 per volume plus shipping and handling. For more information, please contact:

Stephen M. Goodnick
IWCE Chair
Department of Electrical and Computer Engineering
Oregon State University
Corvallis, OR 97331
503-737-2970; 503-737-1300 (FAX)
goodnick@ece.orst.edu

The fourth IWCE will be hosted by Arizona State University in November of 1995.